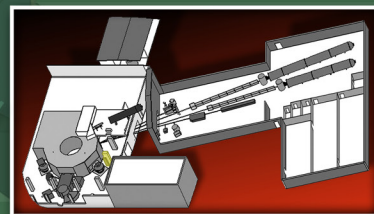


INSTRUMENT

HB-3A

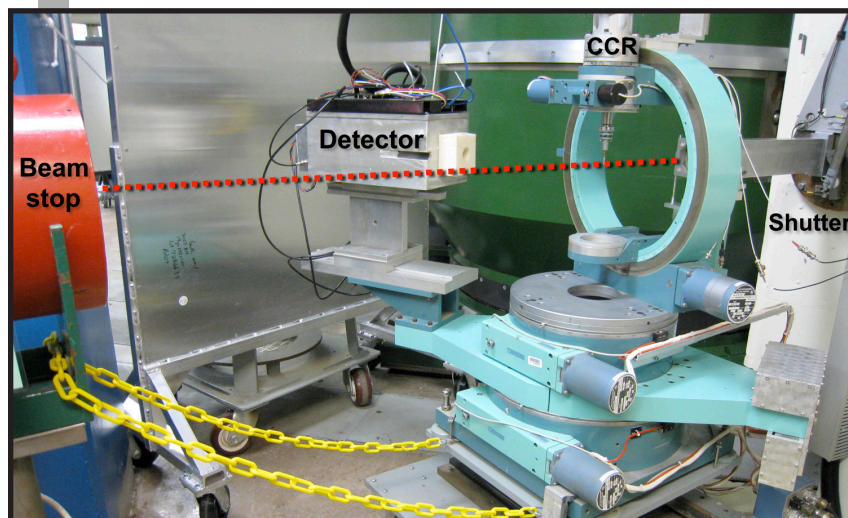
BEAM LINE

HIGH FLUX ISOTOPE REACTOR



FOUR-CIRCLE DIFFRACTOMETER

The Four-Circle Diffractometer goniometer has a full χ circle with a 4-K closed-cycle helium refrigerator. The detector is ^3He with a 7-anode array in a honeycomb pattern. The upper 2θ limit is 95° in bisecting mode. A multilayer-[110]-wafer silicon monochromator with the reflection from planes of the $\langle 011 \rangle$ zone ensures sharp diffraction peaks in specified ranges of detector angles by control of the horizontal radius of curvature. Any plane from the $\langle 011 \rangle$ zone can be set in Bragg position, but only the (331), (220) with (044), and (111) with (333) reflections are of practical interest. For the fixed monochromator angle of 48° , these reflections provide principal incident wavelengths of 1.000, 1.536, and 2.540 Å, respectively. A PC-based system provides user-friendly diffractometer control and data acquisition. The beam size is $5 \times 5 \text{ mm}^2$, and the minimum crystal size is 1 mm^3 . The maximum crystal dimension is about 4 mm. The flux on the sample is up to $2.2 \times 10^7 \text{ n/cm}^2/\text{s}$. Both high-resolution or high-intensity modes are possible by tuning the horizontal bending of the monochromator.



SPECIFICATIONS

Beam spectrum	Thermal
Monochromator	Silicon (fixed vertical flows with adjustable horizontal bending)
Monochromator angle	48°
Incident wavelengths	1.000 Å (331), 1.536 Å (220), 2.5405 Å (111)
Goniometer	Huber, full chi circle, with 4 K CCR
Scattering angles	$2\theta < 95^\circ$ (bisecting mode)
Detector	7 anode ^3He (honeycomb pattern)
Crystal size requirement	$>1 \text{ mm}^3$
Unit-cell size	$<15,000 \text{ Å}^3$
q-resolution	$\Delta q/q \sim 0.01$
Flux at sample	$>2.2 \times 10^7 \text{ n cm}^{-2} \text{ s}^{-1}$

Status: In commissioning

APPLICATIONS

This instrument is suitable for a wide range of small-unit-cell crystallography studies, from structure refinement and solution to charge and nuclear density mapping. Problems from chemistry, physics, materials science, and mineralogy have been addressed. Specific areas of study include hydrogen bonding and weak interactions, organometallics, supramolecular chemistry and crystal engineering, metal hydrides, charge density, pharmaceuticals, and magnetic structures. More general solid-state physics problems in magnetism, diffuse scattering, and ordering phenomena can also be feasible. Unit cell volumes of less than $\sim 7000 \text{ Å}^3$ are practical.

FOR MORE INFORMATION, CONTACT

Instrument Scientist: Huibo Cao, caoh@ornl.gov, 865.253.6078

Instrument Scientist: Bryan Chakoumakos, chakoumakobc@ornl.gov, 865.574.5235

<http://neutrons.ornl.gov/instruments/HFIR/HB3A/>



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